Molecular modeling studies on the binding of Gallic acid to human serum albumin

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Abstract

In this study, the interaction of gallic acid as an anticancer compound with human serum albumin(HSA) was investigated by molecular docking simulation. Binding free energy(ΔG), electrostatic interactions(E_{elec}) and van der waals energies(E_{vdw}) between Gallic acid and HSA were calculated on the basis of force field energy calculations. From the docking simulation the magnitudes of ΔG, E_{elec} and E_{vdw} of gallic acid binding with HSA for the site I (subdomain IIA) were obtained -4.89, -4.47, -1.91, and for site II (subdomain IIIA) they were calculated to be -3.89, -4.17 and -0.7 kcal mol^{-1}, respectively. The results indicated that gallic acid could bind to the site I more stronger than site II of HSA mainly by hydrophobic interaction.

Keyword: HSA, Gallic Acid, Molecular docking